

## **Structure-Activity Relationships for the TMIP Isomers**

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*Ab initio* and semiempirical molecular orbital studies have been carried out for 12 TMIP (2-amino-N,N,N-trimethylimidazo[4,5-b]pyridine) isomers in order to identify the key descriptors of their mutagenic potency. The study of structurally similar heterocyclic amines focuses the search on the electronic properties that influence reactivity. Results will be presented comparing the trends for orbital energies of the parents and nitrenium ions, stability of the nitrenium ions, and electrostatic potentials of the parents to the Ames/*Salmonella* mutagenic activity.

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